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Growth of self-assembled GeSi islands with narrow size distribution on Si (001)

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Abstract. The results of the investigation of the self-assembled Ge islands growth on Si (001) at 700°C are presented. The evolution of the islands shape from "hut" to "dome" islands is studied. For Ge coverage of 11 monolayers a narrow distribution of islands sizes is obtained which allowed to use the Raman spectroscopy and X-ray diffraction for determination of Ge content and residual strain in islands.

Introduction

Elastic stress appearing during the growth of Ge on Si (001) causes a series of morphological changes in the growth front. At submonolayer coverages a $(2 \times n)$ reconstruction forms on film's surface then transforming to (2×8) reconstruction at sufficient Ge amounts (> 1 monolayer (ML)). An increase of Ge coverage (d_{Ge}) up to 3 ML results in elongated two-dimensional islands formation. The next stage of elastic sterss relaxation is formation of three-dimensional (3D) coherent (without dislocations) islands. At some critical islands dimensions the dislocations emerge. The total stress relief occurs by development of a misfit dislocation network. Self-assembled 3D islands have been found to be promising material for Si-based optoelectronics. However, such applications require the islands with the uniform size distribution. Therefore determination of the uniform islands growth conditions is of considerable interest.

In this paper we investigate the growth stages of self-assembled Ge islands deposited on Si(001) at 700°C versus Ge amounts. The growth conditions for uniform islands formation were found. Elastic strain and composition of the islands were measured by Raman spectroscopy and X-ray diffraction.

1 Growth of self-assembled islands

All samples were grown on Si (001) substrates at temperature of 700°C by solid source MBE in a "BALZERS" system. The system was equipped with e-gun for Si and Ge evaporation. The growth rate monitored by the quadrupole mass spectrometer was equal to 1.5 Å/c for Si and 0.15 Å/c for Ge. The samples consist of a 200 nm Si buffer with 1 to 11 ML Ge on top. Atomic force microscopy (AFM) images were recorded in the contact and tapping mode, with "Topometrix"-TMX-2100 AFM and "Solver"-P4 AFM in ambient air.

The onset of Ge islands formation at given growth conditions is observed from AFM images at coverages above 4 ML. At the beginning all islands are the so-called "hut clusters" — well shaped prism-like islands with the bases parallel to the [100] or [010] directions and with {105} facets. At 5.5 equivalent ML of Ge deposited a new kind of islands arises;

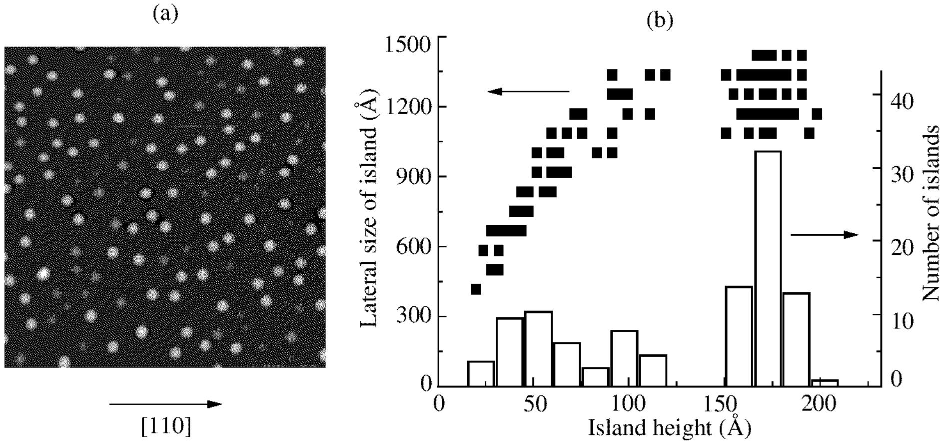

Fig. 1. (a) AFM image (size $2.5 \times 2.5\,\mu m^2$) of the sample with $d_{Ge} = 5.5$ ML; (b) the islands lateral size (D) versus the islands height (H) and histogram of H for this sample.

the so-called "dome-islands" — the islands with fixed lateral size and without clear facets. As an example we show AFM images at 5.5 ML of Ge coverage in Fig. 1(a).

The results of treatment of this image by the special program for determination of the lateral size (D) and height (H) of islands are presented in Fig. 1(b); the bimodal height distribution is clearly seen from the dependence $D(H)$ and from the histogram of the islands height (Fig. 1(b)). We associate the linear relationship on the dependence $D(H)$ with the growth of hut-islands when the lateral size and height of an island increase proportionally. The horizontal region of this dependence corresponds to the growth of dome-islands when the lateral size does not change but the island height gradually increases. From Fig. 2(b) one can estimate the maximal size of hut-islands: $D \approx 1400$ Å, $H \approx 120$ Å. According to the idea suggested in [1] these dimensions define the critical island volume V_c at which the transition from a hut to dome island growth mode occurs. This transition is energetically favourable because at island volume above V_c the dome island energy is less than that of hut-island with the same volume. The chemical potential is decreases step-like in this transition [1], which leads to a rapid growth of dome-islands and to appearance of the bimodal distribution of the island sizes (Fig. 1(b)).

The surface density of islands slightly increases and gradually all hut-islands become dome-ones at an increase of amount of Ge coverage from 5.5 ML to 11 ML. Since dome-islands are of the same lateral size the relative dispersion of D is small (less than 10% at $d_{Ge} = 8$ ML), while the relative dispersion of height distribution is large ($15 \div 20\%$ at the same Ge coverage). An increase of Ge amount up to 11 ML results in remarkable narrowing of both the lateral size and the height distributions (both dispersions are nearly 6%). Such narrow distribution probably results from a local minimum of the dome-islands surface energy or from the energy barrier for generation of dislocation in the islands.

2 Ge content and residual strain in the islands

Determination of Ge content (x) and residual strain (ε) in the islands is important for understanding of their optical properties. However, it is quite difficult to measure either of quantities separately.

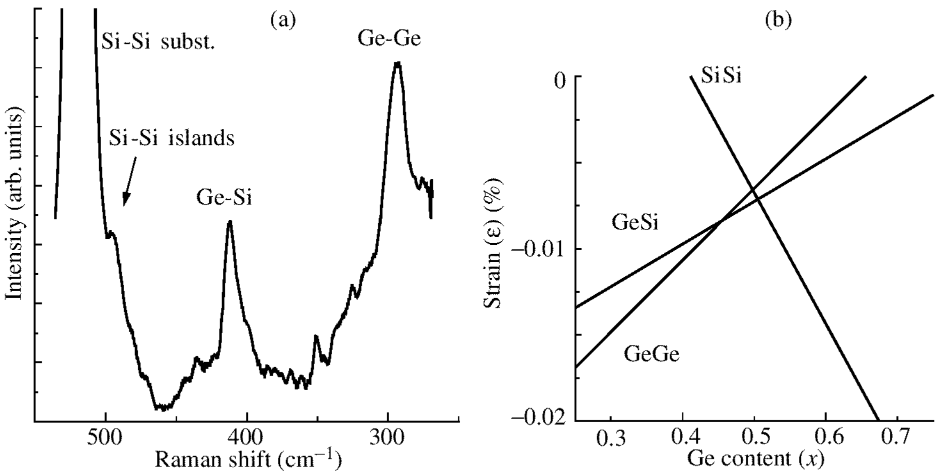

Fig. 2. (a) The Raman spectrum of the sample with $d_{Ge} = 11$ ML; (b) strain (ε) versus Ge content (x) for the sample with $d_{Ge} = 11$ ML.

Uniform islands size distribution in our sample with $d_{Ge} = 11$ ML made it possible to use both the Raman spectroscopy and X-ray diffraction for estimation of x and ε. The Raman scattering and X-ray diffraction measurements were performed at room temperature using DFS-52 spectrometer and DRON-4 diffractometer respectively. Figure 2(a) shows the Raman spectrum of the sample with $d_{Ge} = 11$ ML. Besides the strong Si substrate signal ($\Omega = 520.5\,\mathrm{cm}^{-1}$), the spectrum consists of three peaks which are due to Ge–Ge ($\Omega = 294\,\mathrm{cm}^{-1}$), Si–Ge ($\Omega = 412\,\mathrm{cm}^{-1}$) and Si–Si ($\Omega = 495\,\mathrm{cm}^{-1}$) vibrations [2]. The knowledge of these phonon frequencies allows us to define three linear relationships between x and ε (Fig. 2(b)) [3]. The crossing of any pair of lines in Fig. 2(b) defines a pair of allowed values of x and ε. Note that all the crossing points in Fig. 2(b) are very close to each other. The Ge content and residual strain estimated by this manner are equal to $x = 0.5 \pm 0.05$ and $\varepsilon = -0.7\% \pm 0.05\%$ being in a good agreement with the ones estimated by X-ray diffraction measurements. So one can conclude that at given growth conditions the self-assembled islands at $d_{Ge} = 11$ ML are weakly strained $Si_{0.5}Ge_{0.5}$ alloy. Such a high value of Si content in the islands can not be explained by bulk diffusion of Si at growth temperature especially when the sample does not have a Si cap layer. Thus further experiments are needed for understanding of compositions and strain distribution in self-assembled islands.

Band edges positions of the sample under investigation were calculated using the obtained parameters x and ε [4]. According to this calculations, the energy of the quasi-direct optical transition [4] is about 0.725 eV. A similar structure but with a Si cap layer was investigated by photoluminescence (PL) technique. The peak of PL associated with the islands was observed at the energy of 0.8 eV [4]. The discrepancy between the calculated and the observed values can result from diffusion of Si from the cap layer to the islands and segregation of Ge.

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